Instrumentation Developments

The Advanced Cold Neutron Source

After six years of safe and reliable operation, the liquid hydrogen cold source cryostat at the NIST reactor is being replaced by one with a new advanced design. Based on extensive operating experience and sophisticated Monte Carlo calculations of the cold source and NIST reactor core, the new design improves the neutron coupling between the reactor fuel and moderator and the cold source cryostat. The advanced source, (called Unit 2), will differ from the original in many key respects, as can be seen in Fig. 1. The most important change is the addition of 60 liters of D_2O, partially surrounding the moderator chamber, reducing the moderator void volume and increasing the thermal neutron flux in the cryostat region by about 40 %.

The new cryostat is shaped like an ellipsoidal shell, rather than a spherical one. This results in a smaller volume so that more D_2O can be introduced in the cryostat assembly. The center of the inner ellipsoid is offset, so the liquid hydrogen shell is 30 mm thick near the reactor core. This change results in an additional 5 % to 10 % increase in flux.

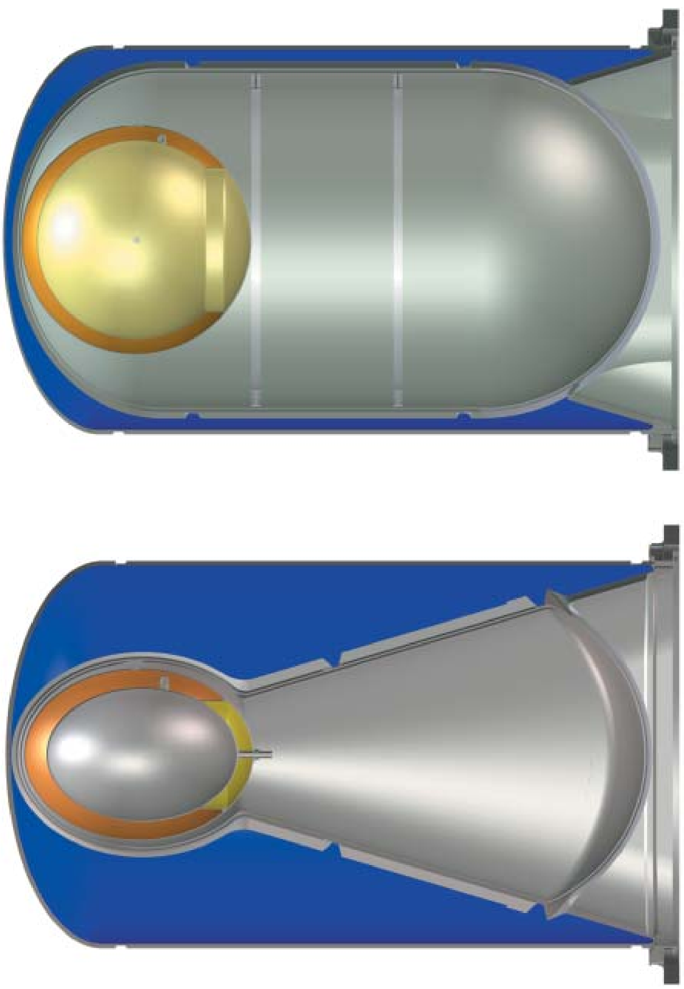

FIGURE 1. Comparison between the original (top) and new designs for the liquid hydrogen cold source cryostat at NIST. Heavy water volume is indicated in blue, liquid hydrogen in orange, and hydrogen vapor in yellow.

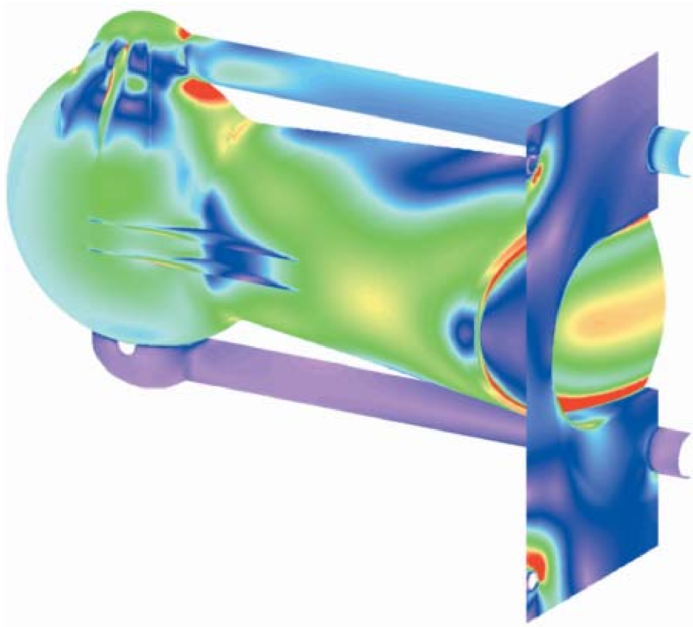

FIGURE 2. False color representation of stresses from finite element calculations of the helium containment jacket with an internal pressure of 82 atmospheres.

Finally, in contrast to the original design, the inner ellipsoid will be evacuated through a small port, removing most of the hydrogen vapor. This change will add another 15 % to 20 % gain. Based on these changes, users can expect an overall intensity increase of 50 % to 80 % between 2 Å and 20 Å with this design.

The complex geometry of the advanced source posed many engineering challenges. The moderator chamber is surrounded by a vacuum vessel, which is surrounded by a helium containment vessel, strong enough to withstand the design basis accidental detonation of liquid hydrogen and solid oxygen. These vessels determine the extent of the D_2O

volume, so they were designed to partially surround the moderator chamber, allowing an opening just large enough to fully illuminate the neutron guides. This "hour-glass" shape created regions of very high mechanical stress, analyzed and ultimately mitigated with the aid of finite element analysis (see Fig. 2). During the three-month period beginning at the end of August 2001, we are removing the old cryostat and installing Unit 2.

Development of an Air-Pad and Floor System for New Neutron Spectrometers

The NCNR is currently developing several new neutron triple axis spectrometers with a key design feature that allows interchangeability of the back-end detector/analyzer systems. Exchanging the back-end system on these instruments requires a universal connection and positioning system between it and the sample position of the instrument. This interface must be capable of achieving an angular accuracy of 0.1 degrees, an angular precision of 0.01 degrees and a vertical positional accuracy of less than a millimeter.

The design approach adopted uses a commercial air-pad system with a precision-leveled floor. After considering several different types of floors we chose to use epoxy as our sub-floor with precision cut and anodized aluminum plates as our contact surface. Epoxy will self-level, fill in holes, and mask over any imperfections in the concrete floor and results in a highly smooth and level surface to build on. The epoxy is also low cost, relatively easy to use, and provides great flexibility for repair or maintenance. The aluminum plates provide protection to the epoxy from cryogenic spills, increased wear resistance, and an easily removable/reusable floor.

FIGURE 3. Michael Murbach and Colin Wrenn conduct tests on the prototype floor system for a triple axis spectrometer.

We have developed and tested a prototype single air-pad system that has successfully demonstrated the construction techniques for the floor system and the ability of the air pad positioning system to meet the accuracy and repeatability requirements for a 1 ton test load. Currently, a three-pad prototype system is under development that will allow us to test control system concepts needed in a final design.

Development of an Intercalated Graphite Monochromator

As part of an ongoing collaboration between NIST and Harvard University to measure the neutron lifetime using magnetically trapped ultracold neutrons (UCNs), a new monochromator has been developed. In the lifetime experiment, ultracold neutrons (UCN: neutrons with energies $\approx$ 100 neV) are produced in a superfluid ^{4}He bath inside the trapping apparatus using the "superthermal process." A beam of cold neutrons is introduced into the helium, in which neutrons with wavelength near 0.89 nm scatter to UCN energies by creation of a single phonon. Only neutrons within a narrow wavelength band ($\pm$ 0.01 nm for our current magnetic trap) participate in this single-phonon production mechanism. Since the wavelength band for UCN production occupies only a small fraction of the neutron spectrum produced by the cold source (see Fig. 4), a significant signal-to-background improvement is possible with appropriate wavelength filtering of neutrons that enter the apparatus. Bragg reflection from a crystalline monochromator with a lattice-plane spacing d can be used to select a narrow wavelength band for neutrons with wavelengths up to $2d$. Unfortunately, widely used materials for neutron monochromatization, such as pyrolytic graphite, have insufficiently large d spacing for reflecting 0.89 nm neutrons. One attractive class of materials for producing long wavelength monochromators is intercalated graphite. Intercalation is the process of inserting foreign atoms or molecules between the layers of the graphite, and results in a crystal with a larger *d* spacing. Intercalated graphites are formed in “stages,” where the stage number defines the number of planes of graphite between layers of intercalant atoms.

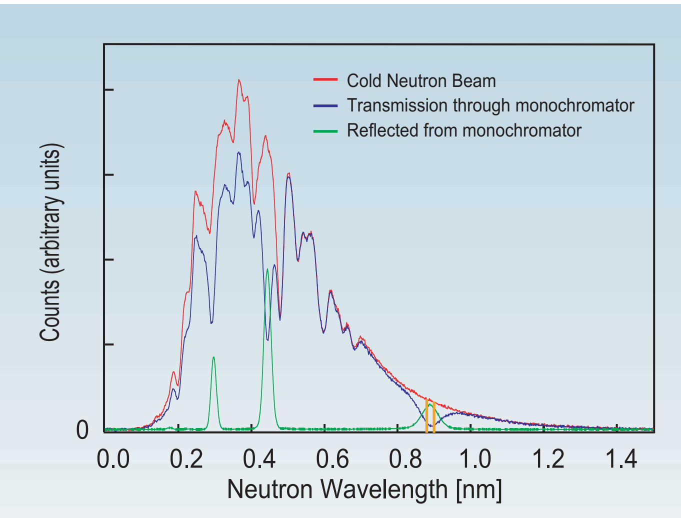

FIGURE 4. Neutron wavelength spectra were measured using a time-of-flight technique. Only 1 % of the neutrons emerging from guide NG-6 (red) lie within the wavelength band (between the orange vertical bars) available for production of UCN. The spectra of neutrons transmitted (blue) and reflected (green) by the monochromator are also shown.

We have designed, fabricated, and tested a new 0.89 nm monochromator using stage-2 potassium-intercalated graphite. Nine pieces of intercalated graphite are tiled to form the monochromator, which has a total size of 6 cm x 15 cm. Heating potassium and graphite to two different temperatures in an evacuated glass cell produces each tile. Performance of the assembled monochromator was determined using time-of-flight techniques (see Fig. 4). The monochromator reflects more than 80 % of the neutrons incident upon it in the wavelength band relevant for UCN production. However, only 3 % of all incident neutrons are reflected. When combined with additional techniques that filter out neutrons from higher order Bragg reflections, the monochromator results in an improvement of the ratio of useful to total neutrons of almost two orders of magnitude while sacrificing few trapped neutrons. During the summer of 2001, this new monochromator was used in conjunction with the trapping apparatus in a temporary setup. Presently, we are permanently installing the monochromator at the fundamental physics station at NG-6. This installation will place the monochromator much closer to the end of the neutron guide and will result in an increase by an additional factor of two in the number of trapped UCNs.

NCNR Computer and Software Environment

The NCNR’s computerized data acquisition and reduction environment encompasses all stages of research: experiment preparation, data collection and analysis of results. NCNR provides site-specific tools that augment the tools in researchers’ own scientific arsenal. Some specific areas of recent activity are described below:

- NCNR is providing simulation tools that model the behavior of our instruments, to evaluate the feasibility of proposed experiments. They can be used by prospective users, especially those who aren’t already familiar with neutron scattering experiments, to explore “what-if” scenarios with different sample and instrument configurations. Currently, we have simulations of small angle scattering experiments, with reflectivity and stress measurement simulations being developed.
- Researchers who plan to use NCNR instrumentation must submit their proposals for review. We have created a web-based proposal submission system that tracks user proposals from submission to review and ranking, to the final instrument time allocation.
- All instruments available at NCNR are computer-controlled. The control software running on these computers must satisfy two seemingly contradictory needs: simplicity, for straightforward use, and sophistication, for power uses. New, more complex instruments, such as the spin echo spectrometer, require carefully designed graphical user interfaces (GUIs) that hide unnecessary detail, while still providing access to all functions, if needed. Since the NCNR instruments run around the clock, the data acquisition functions must be capable of automation and unattended operation. To this end, the experiment control software is scriptable, in addition to the GUI interface. The scriptable, command-based interface fulfills “power-user” needs, while

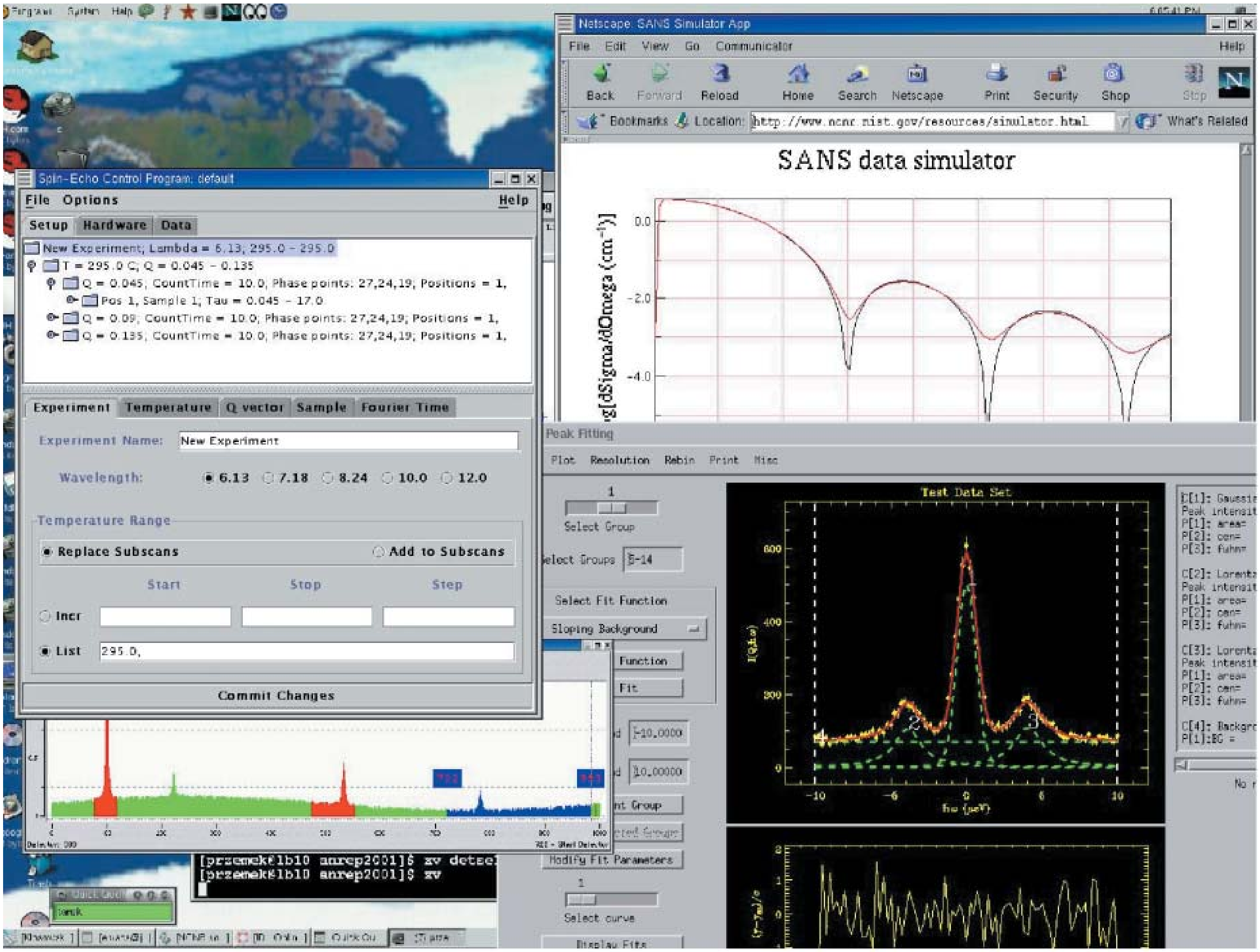

FIGURE 5. A screenshot of several NCNR applications. Clockwise from top left corner: the web-based simulator of a SANS experiment, peak analysis application, Time-of-flight detector selection, and a Spin Echo instrument control panel.

a simplified GUI interface tends to be easier to learn and use.

• Rapid post-acquisition data reduction is important to guide the ongoing experiments, and, later, to aid in the processing of data to obtain the scientific results. Many data reduction procedures are common to all the instruments. The Data Visualization and Analysis Environment (DAVE) is a set of tools commonly used by NCNR scientific community; these tools include programs to manipulate and compare data, extract parameters of theoretical models by data fitting, etc.

• NCNR maintains a sophisticated computer infrastructure including a modern network installation, and an ensemble of nearly 400 computers and other IT equipment, for scientific and office computing, ranging from email servers to supercomputer-style parallel computing clusters.

• NCNR participates in inter-laboratory collaborations developing software for specialized domains. Perhaps the best known of these is the GSAS software for crystallographic data reduction. Another ongoing NCNR collaboration is in international scattering data exchange format, NeXuS.

FIGURE 6. Superconducting magnet/dilution refrigerator as it is being lifted onto the DCS spectrometer. The adjustable lifting frame compensates for the lifting point shifting in case liquid cryogens are added.

Sample Environment Team

The sample environment team expanded by two new members this year, bringing the total number to four employees that are actively working to ensure that the needs of researchers working at the NCNR are met. This team works to improve the infrastructure sample environment equipment and to support neutrons scattering instruments at the NCNR. A principal objective is to provide safe and easy to use equipment to the research staff. Equipment development activities are done in collaboration with the engineering and technical staff, with input from both staff and guest scientists. As an example, a new superconducting magnet/dilution refrigerator system needed modifications for use on the Disk Chopper Spectrometer (DCS) for an experiment. The impracticality of separating the cryostat from its support pumps and electronics led to the decision to lift the entire system onto the instrument for use. A new adjustable lifting frame was design and manufactured to lift the various components of the magnet (see Fig. 6).

Another experiment required the development of a system capable of going to temperatures as high as 675 K with a high voltage applied to the sample. The design goal was to be able to achieve a 5 kV potential difference across the sample. After continued development work, we were able to apply a potential difference of 8 kV to the sample while at the maximum temperature of 675 K. In addition to the human safety features designed in from the beginning, a circuit was developed which prevents the continued arcing that can occur if the sample breaks down during the course of the experiment.